



Materials Models and Simulations for Nuclear Fuels
MMSNF-3, November 18-19, 2004, Washington DC, U.S.A.
Omni Shoreham Hotel, Palladian Ballroom
<http://www.lanl.gov/mst/mmsnf2004/>



THURSDAY, Nov. 18

1:00 PM Session A: Models, Simulations, and Fuel Performance. Chair J. Tulenko (Univ. of Florida)

1:00 M. Stan (LANL) Science-Based Prediction of Nuclear Fuel Properties.

1:20 P. Van Uffelen (ITU), J. Jonnet, and C. Ronchi, *Open Questions Related to the High Burn-up Structure in Nuclear Fuels.*

1:40 W. Liu (MIT), A. Romano, and M. S. Kazimi, *Modeling High-Burnup LWR Fuel Fission Gas Release and Swelling During Fast Transients.*

2:00 S. Shihab (Belgonucleaire), G. Youry, and M. Lippens, *Issues Concerning CERMET Fuel Performance Evaluation with COMETHE.*

2:20 Discussion: *Predictive Methods; Theoretical Versus Empirical.*

2: 40 COFFEE BREAK

3:00 W.T. Thompson (RMC), B.J Lewis, F. Akbari and M. Kaye, *Thermodynamic Modeling of Uranium Oxidation in Support of Defective Fuel Analysis.*

3:20 B.J. Lewis (RMC), W.T. Thompson, J. Higgs, F. Akbari, C. Thurgood, Z. He, R.A. Verrall, and M.R. Floyd, *Modeling of Fuel Oxidation Behavior for Defective Fuel.*

3:40 M. Kato (JNC), K. Konashi, S. Aono, and Y. Kihara, *Model of Oxygen Potential of $(Pu_{0.3}U_{0.7})O_{2\pm x}$ and $(Np_{0.02}Am_{0.02}Pu_{0.3}U_{0.66})O_{2-x}$ Based on Lattice Defect Theory.*

4:00 P. Cristea (LANL), M. Stan, T. C. Wallace, and K. V. Woan, *Controlling Nonstoichiometry of PuO_{2-x} and UO_{2+x} .*

4:20 D. Plancq (CEA), J.M. Ricaud, G.Thouvenin, F. Michel, and V. Marelle, *PLEIADES: A Multi Reactor Simulation Platform for Fuel Performance Modeling.*

4:40 Discussion: *The Perfect Fuel Performance Code; Requirements and Design.*

5:00 PM End of session.

FRIDAY, Nov. 19

8:00 AM Session B: Models, Simulations, and Experimental Validation. Chair K. Pasamehmetoglu (INEL).

8:00 S. P. Rudin (LANL) and J. M. Wills, *First Principles Calculations of the Thermodynamics of ZrN and U.*

8:20 C.R. Stanek (LANL), K.J. McClellan, and R.W. Grimes, *Atomistic Simulation of Actinide Solution and Segregation in UO_2 .*

8:40 B. P. Uberuaga (LANL) and S. M. Valone, *Atomistic Simulations of Ceramics.*

9:00 Z. K. Liu (PennState), *An Integrated Framework for Multi-Component Materials Simulation.*

9:20 Discussion: *Multi-Scale and Multi-Physics Integration.*

9:40 COFFEE BREAK

10:00 E. Copland (NASA) and N. S. Jacobson, *Multiple Effusion-cell Vapor Source Configured Mass Spectrometry and its Application to Thermodynamic Activity Measurements.*

10:20 S. Vogel (LANL), D. Brown B. Clausen, M. Bourke, C. Tome, and Y. Zhao, *Neutrons for Modeling Validation.*

10: 40 K. Katuyama (JNC), S. Miwa, T. Hirose, and K. Tanaka, *Evaluation of Melting Temperature of MOX Fuel Containing Am in JNC.*

11:00 D. Manara (ITU), C. Ronchi, M. Sheindlin, and M. Lewis, *New results on the Melting Behaviour of UO_{2+x} ($0 < x < 0.21$) Through a Novel Experimental Method.*

11:10 H. Seifert (UFL) *Computational Thermodynamics of Nuclear Fuels and their Surrogates.*

11:30 Discussion: *Materials Models and Simulations in Nuclear Fuels Design, Manufacturing, and Operation.*

12:00 PM End of Workshop.

Refreshments will be served. For additional information, please contact Marius Stan (mastan@lanl.gov).